

# Single particle calculations for a Woods-Saxon potential with triaxial deformations, and large Cartesian oscillator basis

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## Abstract

We present a computer program which solves the Schrodinger equation of the stationary states for an average nuclear potential of Woods-Saxon type. In this work, we take specifically into account triaxial (i.e. ellipsoidal) nuclear surfaces. The deformation is specified by the usual Bohr parameters. The calculations are carried out in two stages. In the first, one calculates the representative matrix of the Hamiltonian in the cartesian oscillator basis. In the second stage one diagonalizes this matrix with the help of subroutines of the EISPACK library. If it is wished, one can calculate all eigenvalues, or only the part of the eigenvalues that are contained in a fixed interval defined in advance. In this latter case the eigenvectors are given conjointly. The program is very rapid, and the run-time is mainly used for the diagonalization. Thus, it is possible to use a significant number of the basis states in order to insure a best convergence of the results.

*Key words:* Nuclear physics, Energy levels, Wave functions, Schrodinger equation, Woods-Saxon potential.

*PACS:* code 07.05.Tp, 21.60.-n, 21.60.-cs

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## Program summary

Title of program: Triaxial

Catalogue number:

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Licensing provisions: none

Computer: PC. AMD Athlon 1000MHz

Hard disk: 40 Go

Ram: 256 Mo

Swap file: 4 Go

Operating system: WINDOWS XP

Software used: Microsoft Visual FORTRAN 5.0A (with full optimizations in the settings project options)

Programming language: fortran 77/90 (double precision)

Number of bits in a word: 32

Number of lines: 3150 lines with comments

Keywords: Nuclear physics, Energy levels, Wave functions, Schrodinger equation, Woods-Saxon potential

Nature of the problem:

The Single particle energies and the single particle wave functions are calculated from one-body Hamiltonian including a central field of Woods-Saxon type, a spin-orbit interaction, and the Coulomb potential for the protons.

We consider only ellipsoidal (triaxial) shapes. The deformation of the nuclear shape is fixed by the usual Bohr parameters  $(\beta, \gamma)$ .

Method of solution:

The representative matrix of the Hamiltonian is built by means of the Cartesian basis of the anisotropic harmonic oscillator, and then diagonalized by a set of subroutines of the EISPACK library.

Two quadrature methods of Gauss are employed to calculate respectively the integrals of the matrix elements of the Hamiltonian, and the integral defining the Coulomb potential

Restrictions:

There are two restrictions for the code:

The number of the major shells of the basis does not have to exceed  $N_{\max}=26$ . For the largest values of  $N_{\max}$  ( $\sim 23-26$ ), the diagonalization takes the major part of the running time, but the global run-time remains reasonable.

Typical running time:

(With full optimization in the project settings of the Microsoft Visual Fortran 5.0A on Windows XP )

With NMAX=23, for the neutrons case, and for both parities, if we need all eigenenergies and all eigenfunctions of the bound states, the running time is about 80 sec on the AMD ATHLON computer at 1GHz. In this case, the calculation of the matrix elements takes only about 20 sec.

If all unbound states are required, the runtime becomes larger.

## Long write-up

### 1 Purpose of the Fortran program

#### 1.1 The Schrodinger equation

The program solves the Schrodinger equation for one body-deformed potential:

$$H |\phi_i\rangle = E_i |\phi_i\rangle \quad (1)$$

Here H represents the Hamiltonian of the system (neutrons or protons), and,  $E_i$  , and,  $\phi_i$  , represent respectively, its eigenenergies, and its eigenfunctions.

#### 1.2 The Hamiltonian

The Hamiltonian of the nucleon is defined by [1,2]:

$$H = T + V + V^{so} + e\phi^C \quad (2)$$

The quantities T, V,  $V^{so}$ , indicate respectively, the kinetic, potential , and spin-orbit energy. For the proton, the Coulomb potential is represented by  $\phi^C$  , and  $e$  is its charge

Explicitely:

$$T = -\frac{\hbar^2}{2m} \cdot \vec{\nabla}^2 \quad (3)$$

$\hbar$  = Planck constant

m= nucleon masse

Owing to the fact that the nuclear forces have a short-range character, the average nuclear potential must " follow on average" the nuclear density distribution:

For the case of the spherical symmetry (see also (19)) , we have:

$$V(r) \left( \propto \frac{\rho_0}{1 + \exp(\frac{r-R}{a})} \right) = \frac{V_0}{1 + \exp(\frac{r-R}{a})} \quad (4)$$

For the deformed case, the above definition is generalized as [9]:

$$V(\vec{r}) = \frac{V_0}{1 + \exp(R_V L_V/a_V)} \quad (5)$$

with

$V_0, R_V, a_V$  = mean field parameters

$L_V$  = quasi-radius (see eq. (9))

$$V^{so}(\vec{r}) = -\frac{1}{\hbar} \left( \vec{\nabla} S(\vec{r}) \wedge \vec{p} \right) \vec{\sigma} \quad (6)$$

with

$\vec{p} = (\hbar/i) \vec{\nabla}$  = Neutron or proton momentum

$\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$  = Pauli spin-matrices

For the same reasons that for  $V$ , the mean field in the expression of the  $V^{so}$  operator is given by a similar definition (see also the subsection 3.1) :

$$S(\vec{r}) = \frac{\kappa}{1 + \exp(R_{so} L_{so}/a_{so})} \quad (7)$$

with

$\kappa$  = spin-orbit coupling strength (there, the quantity  $S_0$  is absorbed by  $\kappa$ , this latter is integrated to  $S(\vec{r})$  and expressed in  $MeV.f m^2$ )

$R_{so}, a_{so}$  = mean field parameters of  $S(\vec{r})$

$L_{so}$  is the quasi-radius of the spin-orbit mean field (see eq. (12))

## 2 The Coulomb potential:

For the protons, the Coulomb's potential is approximated by the one of the liquid drop model [1,2]

$$\Phi^C(Z, P, \Phi) = \frac{\rho_{charge}}{4} \int_{Z_1}^{Z_2} dz \times \int_0^{2\pi} d\varphi \left[ \frac{-(z-Z) \frac{\partial \rho_S^2}{\partial z} + 2\rho_S^2 - 2\rho_S P \cos(\varphi - \Phi) - 2P \frac{\partial \rho_S}{\partial \varphi} \sin(\varphi - \Phi)}{\sqrt{(z-Z)^2 + \rho_S^2 + P^2 - 2\rho_S P \cos(\varphi - \Phi)}} \right] \quad (8)$$

where:

$(Z, P, \Phi)$  = cylindrical coordinates of the point where the Coulomb potential is calculated. (here,  $Z$  must not be confused with the protons number)

$\rho_{charge} = (\dot{Z} - 1)e/(4/3)\pi R_{ch}^3$  = charge density of the liquid drop

$(\dot{Z} - 1)$  = "number of protons in the liquid drop"

$R_{ch}$  = radius of the charge density

The integration domain is defined by the volume limited by the surface  $\pi_{ch} = 0$  (see eq. (15)).

The "nuclear surface of the protons" is given by  $\rho_S = \rho_{Surface}$  in the eq. (16). In fact, the code computes directly the quantity  $e\Phi^C$  (which is the Coulomb energy of the proton in the Coulomb field) instead the Coulomb potential  $\Phi^C$ . (see the function *ephi*. in the code).

### 3 Supplementary details on the deformation of the mean field, and the different nuclear surfaces:

#### 3.1 The quasi-radius and the nuclear surfaces

In the central average potential, the information on the distortion of the nuclear surface is given by the dimensionless quasi-radius  $L_V(\vec{r})$ . which is defined as [1]:

$$L_V(\vec{r}) = \frac{\Pi_V(\vec{r})}{R_V \|\vec{\nabla} \Pi_V(\vec{r})\|} \quad (9)$$

The quantity  $\Pi_V(\vec{r})$  is defined so that to recover the well-known spherical case (see section 4).

$$\Pi_V(\vec{r}) = \sqrt{\pi_V(\vec{r}) - \pi_{V \min}} - \sqrt{-\pi_{V \min}} \quad (10)$$

Here,  $\pi_{V \min}$  is the absolute minimum of  $\pi_V(\vec{r})$ . This latter describes an hyper-surface which is not the real nuclear surface, because generally  $\pi_V(\vec{r}) \neq 0$  in the expression of the quasi radius. The actual nuclear surface may be obtained by putting  $\pi_V(\vec{r}) = 0$ .

In this work, we have restricted ourselves only to simple ellipsoidal (triaxial) shapes for the effective nuclear surface.

$$\pi_V(\vec{r}) = \frac{x^2}{A_V^2} + \frac{y^2}{B_V^2} + \frac{z^2}{C_V^2} - 1 = 0 \quad (11)$$

$A_V, B_V$ , and,  $C_V$  are thus the semi-axes of the ellipsoid.

In fact, we have to consider three distinct interactions, i.e. the central, the spin-orbit, and the Coulomb interaction. Therefore, we must define three respective surfaces (equations (11),(14),(15)). Thus, the equation (11) describes

the nuclear surface relatively to the central interaction  $V(\vec{r})$ .

In completely analogous way, we have to define similar quantities for the spin-orbit interaction

$$L_{so}(\vec{r}) = \frac{\Pi_{so}(\vec{r})}{R_{so} \|\vec{\nabla} \Pi_{so}(\vec{r})\|} \quad (12)$$

with,

$$\Pi_{so}(\vec{r}) = \sqrt{\pi_{so}(\vec{r}) - \pi_{so \min}} - \sqrt{-\pi_{so \min}} \quad (13)$$

Where,  $\pi_{so \min}$  is the absolute minimum of  $\pi_{so}(\vec{r})$ , and the effective "spin-orbit surface" is written as:

$$\pi_{so}(\vec{r}) = \frac{x^2}{A_{so}^2} + \frac{y^2}{B_{so}^2} + \frac{z^2}{C_{so}^2} - 1 = 0 \quad (14)$$

For the Coulomb potential, the effective nuclear surface is defined in the same way:

$$\pi_{ch}(\vec{r}) = \frac{x^2}{A_{ch}^2} + \frac{y^2}{B_{ch}^2} + \frac{z^2}{C_{ch}^2} - 1 = 0 \quad (15)$$

Following the expression of the equation (8), the Coulomb potential must be expressed in cylindrical coordinates. Therefore, the equation of the effective "Coulomb nuclear surface" (15) can be rewritten as:

$$\rho_{surface}^2 = \frac{1 - (z/C_{ch})^2}{\{(\cos \varphi/A_{ch})^2 + (\sin \varphi/B_{ch})^2\}} \quad (16)$$

where:

$$x = \rho_{surface} \cos \varphi, \quad y = \rho_{surface} \sin \varphi, \quad z = z$$

The "three densities" (neutrons, protons, spin-orbit) differ very little from each other. Therefore, the three surfaces are homothetic and slightly different to each other. Nevertheless, in order to simplify the problem, the protons distribution is assumed to be uniform in the calculation of the Coulomb potential.

### 3.2 The deformation parameters

Since we have three similar surfaces, and, so as to avoid repeating three times the same thing, we will omit to specify the indices of the surfaces. For example, the three volume conservation conditions are simply replaced by only one equation :

$$\frac{4}{3}\pi ABC = \frac{4}{3}\pi R^3 \quad (17)$$

Actually, because of this condition, only two parameters are necessary

As usual, one will prefer the Bohr parameters  $(\beta, \gamma)$  instead of those of the

ellipsoid.

$$A = \frac{R}{\chi} \left[ 1 + \beta \left( \frac{5}{4\pi} \right)^{1/2} \cos\left(\gamma - \frac{2}{3}\pi\right) \right] \quad (18a)$$

$$B = \frac{R}{\chi} \left[ 1 + \beta \left( \frac{5}{4\pi} \right)^{1/2} \cos\left(\gamma - \frac{4}{3}\pi\right) \right] \quad (18b)$$

$$C = \frac{R}{\chi} \left[ 1 + \beta \left( \frac{5}{4\pi} \right)^{1/2} \cos(\gamma) \right] \quad (18c)$$

$R$  is the radius, and,  $\chi$  insures the volume conservation condition (17),

## 4 The Spherical case. The mean field parameters

### 4.1 The case of spherical symmetry

When  $A=B=C$ , or when the Bohr parameter  $\beta = 0$ , the nuclear surface becomes spherical, and  $R_V$ ,  $R_{so}$ , or,  $R_{ch}$  represents simply the nucleus radius. In this case, we obtain the familiar Fermi-function for the two mean potentials ((5),(7)):

$$V(\vec{r}) = \frac{V_0}{1 + \exp[(r - R_V)/a_V]} \quad S(\vec{r}) = \frac{\kappa}{1 + \exp[(r - R_{so})/a_{so}]} \quad (19)$$

i.e. potentials of Woods-Saxon type.

The Coulomb's potential (8) reduces to the well-known form:

$$\begin{aligned} \Phi^c(r) &= [(Z - 1)e/2R_{ch}] [3 - (r/R_{ch})^2] \quad \text{if} \quad r \leq R_{ch} \\ \Phi^c(r) &= (Z - 1)e/r \quad \text{if} \quad r \geq R_{ch} \end{aligned} \quad (20)$$

The spin-orbit interaction (6) can be expressed in the spherical case as:

$$V^{so} = -\left(\frac{\partial S(r)}{\partial r} \frac{\vec{r}}{r} \wedge \vec{p}\right) \vec{\sigma} = -\frac{1}{r} \frac{\partial S(r)}{\partial r} (\vec{r} \wedge \vec{p}) \vec{\sigma} \quad (21)$$

Finally, the  $V^{so}$  operator takes the familiar form,

$$V^{so}(\vec{r}) = -\frac{1}{r} \frac{\partial S(r)}{\partial r} \vec{l} \cdot \vec{\sigma} \quad (22)$$

The relations (19-22) of the spherical case are not used explicitly in the code. However, the well known spherical degeneracy of the energy levels were used

in order to check the program. Moreover, the relation (20) serves as a first checking for the Coulomb potential.

## 4.2 Mean field parameters

Two options have been included in the code in order to choose between a particular set of parameters, or the Myers parameters [3]. Thus, it is possible to define its own parameters in a separate file, or to employ those of Myers. In this latter case, the calculations are made in a suitable subroutine. In fact, only a part of the parameters set, namely,  $V_0, R_V, R_{so}, R_{ch}$ , is deduced from the droplet model of Myers, the remaining, i.e.  $\kappa, a_V, a_{so}$ , are extracted from the Ref. [1]. The explicit expressions for these parameters are given in appendix.

# 5 Principle of resolution

## 5.1 The method

The principle of this method consists to look for the eigenfunctions of the Schrodinger equation by their expansion on a truncated basis of the harmonic oscillator. In other words, the method used in solving such problem amounts essentially to writing the representative matrix of the Hamiltonian in this basis.

In practice, this method is characterized by two distinct stages. First, one builds the representative matrix of the Hamiltonian by means of the cited basis. Next, one diagonalizes this matrix in order to obtain the eigenvalues and the eigenvectors.

In our work, the cartesian coordinates are the most suitable.

## 5.2 The harmonic oscillator basis

The basis functions of the harmonic oscillator are defined as:

$$|n_x n_y n_z \Sigma\rangle \equiv i^{n_y} \phi_{n_x}(x) \cdot \phi_{n_y}(y) \cdot \phi_{n_z}(z) \cdot \vec{\sigma}_\Sigma \quad (23)$$

There,  $i^{n_y}$  is a phase factor which insures, in accordance with the imposed symmetries (see section 6), that the matrix elements are real.



Explicitly:

$$\phi_{n_x}(x) = \sqrt{\beta_x} \exp \left[ -(\beta_x x)^2 / 2 \right] \cdot h_{n_x}(\beta_x x) \quad \text{with} \quad \beta_x = \sqrt{\frac{m\omega_x}{\hbar}} \quad (24)$$

with analogous expressions for the y, and z axes.

The intrinsic spin states are:

$$\vec{\sigma}_{+1/2} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \vec{\sigma}_{-1/2} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (25)$$

The  $h_{n_x}$ , (or  $h_{n_y}$ , or  $h_{n_z}$ ) quantities symbolize the normalized Hermite polynomials.

$$h_{n_x}(x) = H_{n_x}(x) / \sqrt{(2^{n_x} \cdot n_x! \pi^{1/2})} \quad (26)$$

$H_{n_x}(x)$  are the usual Hermite polynomials

The quantum numbers  $n_x$ ,  $n_y$ ,  $n_z$ , are integers, and give the order of the Hermite polynomials,  $\Sigma = \pm \frac{1}{2}$  represents the projection of the intrinsic spin on the z-axis.

At last,  $m$  and  $\omega_x$ ,  $\omega_y$ ,  $\omega_z$  represents the mass of the oscillator, i.e. the mass of the nucleon, and, its frequencies.

For convenient, the quantities  $\hbar\omega_x$ ,  $\hbar\omega_y$ ,  $\hbar\omega_z$ , (or respectively  $\beta_x, \beta_y, \beta_z$ ) are called the deformation parameters of the basis.

If the three frequencies are equal, the oscillator is then isotropic, and it can be characterized by only one frequency ( $\omega_x = \omega_y = \omega_z = \omega_0$ )

Furthermore, we assume that the nuclear surface of the oscillator is an equipotential. This involves the following condition:

$$\omega_x \omega_y \omega_z = \omega_0^3 \quad \text{or} \quad (\hbar\omega_x) \cdot (\hbar\omega_y) \cdot (\hbar\omega_z) = (\hbar\omega_0)^3 \quad (27)$$

### 5.3 The representative matrix of the Hamiltonian

With help of this basis, the matrix elements of the Hamiltonian  $H$  can be written as:

$$\langle n'_x n'_y n'_z \Sigma' | H | n_x n_y n_z \Sigma \rangle = \langle n'_x n'_y n'_z \Sigma' | T + V + V^{so} + e \cdot \Phi^c | n_x n_y n_z \Sigma \rangle \quad (28)$$

### 5.3.1 Matrix elements of the mean field $V$ and the Coulomb energy $e.\Phi^C$

Since  $V$  does not depend on the spin, we adopt the following convenient notation for  $V$ :

$$\langle n'_x n'_y n'_z \Sigma' | V | n_x n_y n_z \Sigma \rangle = \left( n'_x n'_y n'_z | V | n_x n_y n_z \right) \times \delta_{\Sigma' \Sigma} \quad (29)$$

where:

$$\begin{aligned} & \left( n'_x n'_y n'_z | V | n_x n_y n_z \right) \\ &= i^{(n_y - n'_y)} \iiint \phi_{n'_x}(x) \phi_{n'_y}(y) \phi_{n'_z}(z) V(x, y, z) \phi_{n_x}(x) \phi_{n_y}(y) \phi_{n_z}(z) dx dy dz = \\ &= i^{(n_y - n'_y)} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{-(x^2 + y^2 + z^2)} h_{n'_x}(x) . h_{n'_y}(y) . h_{n'_z}(z) \\ &\quad \times V\left(\frac{x}{\beta_x}, \frac{y}{\beta_y}, \frac{z}{\beta_z}\right) . h_{n_x}(x) . h_{n_y}(y) . h_{n_z}(z) . dx dy dz \quad (30) \end{aligned}$$

with  $\beta_x, \beta_y, \beta_z$  defined in eq.(24)

- Due to the parity of  $V$ , the integral (30) vanishes if one of the three following conditions is not fulfilled:

$$\begin{aligned} (-1)^{n_x} &= (-1)^{n'_x} \\ (-1)^{n_y} &= (-1)^{n'_y} \\ (-1)^{n_z} &= (-1)^{n'_z} \end{aligned}$$

Therefore, it is not necessary to calculate them.

Since the respective indices must have the same parity, the complex factor of (30) can be rewritten as:

$$i^{(n'_y - n_y)} = (-1)^{(n'_y - n_y)/2}$$

- Although the  $\left( n'_x n'_y n'_z | V | n_x n_y n_z \right)$  elements are spin independent, they are stored actually as:  $\langle n'_x n'_y n'_z \Sigma' | V | n_x n_y n_z \Sigma \rangle$  in the computer memory
- The matrix elements of the Coulomb energy are calculated in the same way as those of  $V(\vec{r})$  (putting  $e\phi^c(\vec{r})$  instead  $V(\vec{r})$ ), with the same change of scale.
- In the gaussian integration, we have to calculate the Hermite polynomials, the central mean potential  $V(\vec{r})$ , the spin-orbit mean potential  $S(\vec{r})$ , and the Coulomb potential  $\phi^c(\vec{r})$  only at the nodes. Therefore, it is more convenient to store these quantities in specific arrays before any calculations (see the common/tabh/... declaration in the subroutine setsub).

### 5.3.2 Matrix elements of the spin-orbit energy operator $V^{so}$

Due to the presence of the derivative of  $S(\vec{r})$ , the direct calculation of the matrix elements of  $V^{so}$ , i.e.  $\langle n'_x n'_y n'_z \Sigma' | V^{so} | n_x n_y n_z \Sigma \rangle$ , is not convenient. These derivatives can be transferred on the basis functions by partial integration. Therefore, the derivatives of the basis functions can be expressed from the basis functions themselves by mean of the recursion relations. Finally, the matrix elements of  $V^{so}$  can be obtained by suitable combinations of  $(n'_x n'_y n'_z | S | n_x n_y n_z)$  elements, i.e.

$$\begin{aligned} \langle n'_x n'_y n'_z \Sigma' | V^{so} | n_x n_y n_z \Sigma \rangle = \\ \frac{m\omega_0}{2\hbar} [2B_z (\Sigma' | \sigma_z | \Sigma) + B_+ (\Sigma' | \sigma_- | \Sigma) + B_- (\Sigma' | \sigma_+ | \Sigma)] \end{aligned} \quad (31)$$

where:

$$\sigma_{\pm} = \sigma_x \pm \sigma_y \quad (32)$$

$$B_{\pm} = B_x \mp B_y \quad (33)$$

$$\begin{aligned} B_x = \sqrt{\frac{\omega_y \omega_z}{\omega_0^2}} & [-\sqrt{n'_y(n_z + 1)} (n'_x n'_y - 1, n'_z | S | n_x n_y n_z + 1) \\ & - \sqrt{n_y(n'_z + 1)} (n'_x n'_y n'_z + 1 | S | n_x n_y - 1, n_z) \\ & + \sqrt{n_z(n'_y + 1)} (n'_x n'_y + 1, n'_z | S | n_x n_y n_z - 1) \\ & + \sqrt{n'_z(n_y + 1)} (n'_x n'_y, n'_z - 1 | S | n_x n_y + 1, n_z)] \end{aligned} \quad (34)$$

$$\begin{aligned} B_y = \sqrt{\frac{\omega_z \omega_x}{\omega_0^2}} & [-\sqrt{n'_z(n_x + 1)} (n'_x, n'_y n'_z - 1 | S | n_x + 1, n_y n_z) \\ & + \sqrt{n_z(n'_x + 1)} (n'_x + 1, n'_y n'_z | S | n_x n_y n_z - 1) \\ & - \sqrt{n_x(n'_z + 1)} (n'_x n'_y n'_z + 1 | S | n_x - 1, n_y, n_z) \\ & + \sqrt{n'_x(n_z + 1)} (n'_x - 1, n'_y n'_z | S | n_x n_y n_z + 1)] \end{aligned} \quad (35)$$

$$\begin{aligned}
B_z = \sqrt{\frac{\omega_x \omega_y}{\omega_0^2}} & [-\sqrt{n'_x(n_y + 1)} (n'_x - 1, n'_y n'_z |S| n_x n_y + 1, n_z) \\
& - \sqrt{n_x(n'_y + 1)} (n'_x n'_y + 1 n'_z |S| n_x - 1, n_y n_z) \\
& + \sqrt{n_y(n'_x + 1)} (n'_x + 1, n'_y n'_z |S| n_x n_y - 1, n_x) \\
& + \sqrt{n'_y(n_x + 1)} (n'_x n'_y - 1, n'_x |S| n_x + 1, n_y n_x)
\end{aligned} \tag{36}$$

where  $S(\vec{r})$  is given by eq.(7)

- The changes of sign in  $B_y$  are involved by the phase factor of the basis functions.
- The computations of the matrix elements of  $S(\vec{r})$  are carried out like those of  $V(\vec{r})$  in (30).

### 5.3.3 Matrix elements of the kinetic energy operator $T$

At last, the matrix elements of the  $T$  operator can be calculated in straightforward way:

$$\begin{aligned}
\langle n'_x n'_y n'_z \Sigma' | T | n_x n_y n_z \Sigma \rangle &= \frac{1}{4} \delta_{\Sigma \Sigma'} i^{(n_y - n'_y)} \times \\
& [\hbar \omega_z \delta_{n_x n'_x} \delta_{n_y n'_y} \delta_{n_z n'_z} (2n_z + 1) \\
& - \hbar \omega_z \delta_{n_x n'_x} \delta_{n_y n'_y} \delta_{n_z n'_z + 2} \sqrt{n'_z(n_z + 1)} \\
& - \hbar \omega_z \delta_{n_x n'_x} \delta_{n_y n'_y} \delta_{n_z n'_z - 2} \sqrt{n_z(n'_z + 1)} \\
& + \text{cyclic permutations}]
\end{aligned} \tag{37}$$

## 6 Symmetry properties of the nuclear surface

The three surfaces can be written as:

$$\pi = \frac{x^2}{A^2} + \frac{y^2}{B^2} + \frac{z^2}{C^2} - 1 = 0 \tag{38}$$

This implies the following properties:

$$\pi(x, y, z) = \pi(-x, y, z) = \pi(x, -y, z) = \pi(x, y, -z) \tag{39}$$

Thus, for the two mean fields (i.e. central and spin-orbit fields), and for the Coulomb potential, we obtain:

$$V(-x, -y, -z) = V(x, y, z) \quad (40)$$

$$S(-x, -y, -z) = S(x, y, z) \quad (41)$$

$$\Phi^C(-x, -y, -z) = \Phi^C(x, y, z) \quad (42)$$

### 6.1 Parity

Because of the relations (40), (41), and (42) the parity is a good quantum number, and the initial matrix decays into two sub-matrices according to the number

$$p_a = (-1)^{n_x+n_y+n_z} = \pm 1 \quad (43)$$

Obviously, if  $(n_x + n_y + n_z)$  is even or odd the parity is respectively positive or negative.

### 6.2 Signature

Furthermore, the Kramers degeneracy is expressed here, by the fact that the eigenvalues are doubly degenerated relatively to the signature quantum number  $q_K$ , which is defined by:

$$q_K = (-1)^{n_x+n_y}\Sigma = \pm 1/2 \quad (44)$$

Consequently, the secular matrix splits into two sub-matrices, and only one must be considered. The two matrices contain the same set of eigenvalues, but the eigenfunctions are time-reversed each other.

### 6.3 Consequences of these symmetries

The computer code carries out calculations only for one kind of particles. Therefore, in order to take into account both neutrons and protons, the code must be run twice.

Since the Hamiltonian connects only states with the same parity, the computer code is built in such way that it separates the two types of parity  $p_a = \pm 1$  and performs the calculations separately for them. Consequently, the representative matrix of the Hamiltonian splits into two blocks with a definite parity for each block. The diagonalization is then carried out in each block.

Furthermore, the Kramers degeneracy involves the same eigenvalues for states which are time-reversed each other. For each block of a definite parity, the eigenenergies can be separated into two sets defined by the signature  $q_K = \pm 1/2$ . The code will make calculations only for  $q_K = +1/2$ . The second block  $q_K = -1/2$  will be implicit, and will contain same energies but with time-reversed eigenfunctions. These eigenvectors may be obtained by application of the time reversal operator, i.e. by the operator  $T = -i\sigma_y K_0$ , where  $\sigma_y$  is a Pauli matrix and  $K_0$  is the operator of complex conjugation.

Thus, one obtains 8 blocks, of which 4 are actually calculated (i.e. here the four first).

- 1)  $[n] \quad [p_a = +1] \quad [q_K = +1/2]$
- 2)  $[n] \quad [p_a = -1] \quad [q_K = +1/2]$
- 3)  $[p] \quad [p_a = +1] \quad [q_K = +1/2]$
- 4)  $[p] \quad [p_a = -1] \quad [q_K = +1/2]$
- 5)  $[n] \quad [p_a = +1] \quad [q_K = -1/2]$
- 6)  $[n] \quad [p_a = -1] \quad [q_K = -1/2]$
- 7)  $[p] \quad [p_a = +1] \quad [q_K = -1/2]$
- 8)  $[p] \quad [p_a = -1] \quad [q_K = -1/2]$

So, it is important to point out that, the number of the basis states practically taken into account by the code is the half of the actual number.

## 7 Numerical choices and prescriptions

### 7.1 The quadratures

The matrix elements of  $V(\vec{r})$ ,  $e\Phi^C(\vec{r})$  and  $V^{so}(\vec{r})$  are calculated with the Gauss-Hermite method, with  $30 \times 30 \times 30$  of mesh points. The Coulomb potential  $\Phi^C(\vec{r})$  is also evaluated numerically by the Gauss-Legendre method, but with  $48 \times 48$  of mesh points.

These choices seem to be sufficient relatively to the size of the basis ( $N_{\max} \leq 26$ ), and the interval of deformation ( $0 \leq \beta \leq 0.6$ ). A direct checking has

been done by increasing the number of quadrature points and by comparing the stability of the results (even with 20 points the results remain very correct).

## 7.2 Prescription of the basis truncation

In practice, the Hamiltonian matrix is finite. Therefore, for reasons of accuracy, we have to select a sufficient number of the basis states. Generally, we adopt one of the two following criteria:

The first (spherical criterion) consists in choosing all basis states which satisfy the following inequality.

$$n_x + n_y + n_z \leq N_{\max} \quad (45)$$

With this criterion the total number of the basis states is given by  $(N_{\max}+1) \times (N_{\max}+2) \times (N_{\max}+3)/6$ .

In the second criterion (deformed criterion), one selects the states according to the deformation of the basis, i.e. according to the three frequencies of basis.

$$(n_x + \frac{1}{2})\hbar\omega_x + (n_y + \frac{1}{2})\hbar\omega_y + (n_z + \frac{1}{2})\hbar\omega_z \leq E_{cut} = (N_{\max} + \frac{3}{2})\hbar\omega_0 \quad (46)$$

(In fact, these three frequencies are already connected by the condition (27)). Thus, the choice of  $N_{\max}$  determines the size of the basis. The files "conver12.res" and "conver13.res" give some details about this.

## 7.3 Optimization of the basis frequencies

Since the Hamiltonian operator does not depend on the oscillator frequencies, its eigenfunctions, and its eigenenergies, must not depend on these parameters. In practice, the representative matrix of the Hamiltonian is built by means of a finite number of oscillator eigenfunctions. This implies a *spurious* dependence according to these parameters.

In another point of view, we might consider this method as a variational method in which the variational parameters are the frequencies of the basis. Thus, the best set (in terms of energy) for these frequencies should be precisely the one, *which minimizes the eigenenergies*, or simply their sum.

For practical reasons, this method is not easy, since the variation is three-dimensional. However, it can be often more efficient to use some prescriptions in order to find (in an economical way) suitable values for these parameters. In the present work, we have adopted the approach of the references [1] and

[9]. In that method, we define first, the quantities  $p$  and  $q$  by:

$$q^2 = \frac{\langle z^2 \rangle}{\langle x^2 \rangle} = \frac{\int d\tau \cdot \rho(\vec{r}) z^2}{\int d\tau \cdot \rho(\vec{r}) x^2} \quad p^2 = \frac{\langle z^2 \rangle}{\langle y^2 \rangle} = \frac{\int d\tau \cdot \rho(\vec{r}) z^2}{\int d\tau \cdot \rho(\vec{r}) y^2} \quad (47)$$

where  $\rho(\vec{r})$  is the nuclear density. Note that the present definition of  $p$  differs from that of the ref.[1].

For a harmonic oscillator, the equations (47) are reduced to very simple relations.

$$q_{HO} = \frac{\omega_x}{\omega_z} \quad p_{HO} = \frac{\omega_y}{\omega_z} \quad (48)$$

Next, we have to add, to these two formulas, the relation (27). Now, it is possible to replace the parameter set  $(\omega_x, \omega_y, \omega_z)$  by the equivalent  $(q_{HO}, p_{HO}, \omega_0)$ . In the same way, for the potential of Woods-Saxon, the nuclear density can be approximated by the one of the liquid drop (i.e. a constant density). We obtain thus:

$$q_{WS} = \frac{c}{a} \quad p_{WS} = \frac{c}{b} \quad (49)$$

At last, we “adapt” the oscillator basis to the nuclear shape by requiring:

$$q_{HO} = q_{WS} \quad p_{HO} = p_{WS} \quad (50)$$

For the  $\omega_0$  value, we can adopt simply the one of the Nilsson model.

$$\hbar\omega_0 \approx 41.A^{-\frac{1}{3}} \quad (51)$$

Many tests have shown that relations (50) and (51) give *automatically* very close values to those that produce the “true” minimization. Furthermore, a general rule is that a large basis size involves always a weak dependence of the eigenvalues according to these parameters. Going to the limit, we can say that if the basis was infinite, the results would be independent to the basis parameters. Conversely, for a too small basis, the dependence is strong, and the results become too inaccurate.

For a square well, or (approximately) a Woods-Saxon potential, simple analytical considerations lead to a more “refined” value for the parameter  $\hbar\omega_0$ :

$$\hbar\omega_0 \approx \frac{5}{3} \left( \frac{2}{\pi^2} \right)^{1/3} |V_0| . A^{-1/3} \approx 0.979 |V_0| . A^{-1/3} \quad (52)$$

where  $V_0$  is the depth of the potential. The equation (52) is obtained by requiring the condition

$$\langle r^2 \rangle_{\text{harm. Oscillator}} = \langle r^2 \rangle_{\text{square well}}$$

The averages are made with the semi-classical Thomas-Fermi density:

$$\rho_{TF}(r) = \frac{(2m)^{3/2}}{3\pi^2\hbar^3} (\lambda - V(r))^{3/2}$$



The Fermi level  $\lambda$  is determined by the condition of conservation of the particle number  $A$ .

The relation (52) could explain the empirical scale factor used sometimes [1,2,5] in the "standard equation" (51).

#### 7.4 The numerical values of the $\beta$ parameters of the basis

The quantities  $\beta_0 = \sqrt{\frac{m\omega_0}{\hbar}}$ ,  $\beta_x = \sqrt{\frac{m\omega_x}{\hbar}}$ ,  $\beta_y = \sqrt{\frac{m\omega_y}{\hbar}}$ , and  $\beta_z = \sqrt{\frac{m\omega_z}{\hbar}}$  are numerically calculated like

$$\sqrt{\frac{m\omega}{\hbar}} = \sqrt{\frac{mc^2}{\hbar^2 c^2}} \hbar \omega$$

The values are:

$$m_p c^2 = 938.2592 \text{ MeV}$$

$$m_n c^2 = 939.553 \text{ MeV}$$

$$\hbar c = 197.32879 \text{ MeV fm}$$

This involves:

$$\frac{m_p c^2}{(\hbar c)^2} = t_p = 0.0240958315 \text{ MeV}^{-1} \text{ fm}^{-2} \quad (53)$$

$$\frac{m_n c^2}{(\hbar c)^2} = t_n = 0.0241290571 \text{ MeV}^{-1} \text{ fm}^{-2} \quad (54)$$

so that :

$$\beta_0 = \sqrt{t \cdot \hbar \omega_0}, \quad \beta_x = \sqrt{t \cdot \hbar \omega_x}, \quad \beta_y = \sqrt{t \cdot \hbar \omega_y}, \quad \beta_z = \sqrt{t \cdot \hbar \omega_z} \quad (55)$$

with  $t = t_p$  or  $t = t_n$

The numbers  $t_p$  and  $t_n$  appear in the subroutine "Basisparam".

## 8 Diagonalization

The diagonalization of the representative matrix of the Hamiltonian is carried out by a set of subroutines extracted from the EISPACK library of FORTRAN programs (<http://www.netlib.org/eispack/>). Thus, four subroutines of this library were gathered:

The subroutine tred1 transforms any full symmetrical matrix into a tridiagonal symmetrical matrix by using the Givens-Householder's method.

For a tridiagonal symmetrical matrix the subroutine tq11 uses the ql method to calculate only the eigenvalues of a tridiagonal matrix.

For a tridiagonal symmetrical matrix, the subroutine *tsturm* calculates the eigenvalues contained in a given interval. This subroutine calculates also the eigenvectors associated to the found eigenvalues. The adopted method is that of the bisection and the inverse iteration.

Lastly, the subroutine *trbak1* recalculates the eigenvectors found by *tsturm* relatively to the initial basis (that of *tred1*). The sought eigenvectors are thus obtained.

These subroutines are called by the subroutines *diagoplus* (for the positive parity), and *diagominus* (for the negative parity) in which the options of the diagonalization are specified. These options are indicated in the comments of the program, and below, in the subsection 10.1.1.

## 9 The subroutines and the functions of the Program.

The program is composed by a main program, 29 subroutines and 6 functions. The role reserved for each program is briefly described in the paragraph below (and described again in details in the comments of the program).

In fact, all calculations are governed by the subroutine *setsub* which is in some sense a super subroutine.

### 9.1 The set of subroutines (in the order of the calls)

- (1) The subroutine *read1*: reads the basic input parameters in the file *input.dat*
- (2) The subroutine *write1*: performs some tests and writes on a files *eigvals.res* and *conver.res*
- (3) The subroutine *setsub*: drives the successive calculations
- (4) The subroutine *write2*: writes on the file *eigvals.res*
- (5) The subroutine *write3*: writes on the file *conver.res*
- (6) The subroutine *woodsparam*: calculates the Myers parameters
- (7) The subroutine *surfparam*: calculates the surfaces parameters
- (8) The subroutine *basisparam*: calculates the oscillator basis parameters
- (9) The subroutine *pottablo* : stores the potential at the nodes of quadrature
- (10) The subroutine *coefftablo*: stores the products of the coefficient of quadrature
- (11) The subroutine *hermitablo*: stores the Hermite polynomials at the nodes
- (12) The subroutine *coultablo*: stores the coulomb potential at the nodes
- (13) The subroutine *statesplus*: selects the numbers and the oscillator basis states corresponding to the positive parity
- (14) The subroutine *statesminus*: selects the numbers and the oscillator basis states corresponding to the negative parity
- (15) The subroutine *idm*: calculates the total numbers of the used basis states

- (16) The subroutine *matpotplus*: calculates the representative matrix of the central mean potential for the positive parity
- (17) The subroutine *matpotminus*: calculates the representative matrix of the central mean potential for the negative parity
- (18) The subroutine *matcinplus*: calculates the representative matrix of the kinetic energy for the positive parity
- (19) The subroutine *matcinminus*: calculates the representative matrix of the kinetic energy for the negative parity
- (20) The subroutine *matpotsoplus*: calculates the representative matrix of the mean spin-orbit energy for the positive parity
- (21) The subroutine *matpotsominus*: calculates the representative matrix of the mean spin-orbit energy for the negative parity
- (22) The subroutine *diagoplus*: diagonalizes the representative matrix of the hamiltonian for the positive parity
- (23) The subroutine *diagominus*: diagonalizes the representative matrix of the hamiltonian for the negative parity
- (24) The subroutine *tred1*: Eispack subroutine (see section 8)
- (25) The subroutine *tql1*: Eispack subroutine (see section 8)
- (26) The subroutine *tsturm*: Eispack subroutine (see section 8)
- (27) The subrouine *trbak1*: Eispack subroutine (see section 8)
- (28) The subroutine *eigenvalues*: gathers the eigenvalues for both parities
- (29) the subroutine *vektors*: writes the eigenfunctions in a file.

Fore several subroutines, the names ending in “plus” or in “minus” means that the subroutine performs calculations specifically for a defined parity. The term “plus” is employed for the positive parity, and the term “minus” for the negative parity.

## 9.2 The set of functions

- (1) The function *Hermite*: calculates the Hermite polynomials
- (2) The function *delta*: delta symbol of Kroneker
- (3) The function *potenv*: calculates the central mean potential value at any point.
- (4) The function *potenso*: calculates the spin-orbit mean potential value at any point.
- (5) The function *ephi*: calculates the Coulomb energy of the proton at any point.
- (6) The function *epsilon*: estimates the round-off error for the Eispack subroutines

## 10 Input-output data of the FORTRAN program

If no modifications are made the use of the program as presented in long theoretical description is very simple.

### 10.1 The input data

All input data are read from two files in a namelist type declarations. The second file is needed only if one does use a personal parameters for the potential, instead those of Myers. In this latter case, one has to precise its own parameters, in a second separate file.

#### 10.1.1 The first input data file: input.dat

The file input.dat gathers all basic input data. Their significance is given below.

- $nmax1$  and  $nmax2$  are the bounds of the loop for  $N_{\max}$  (eq(45) or (46)). This latter is the number of the major shells used in the calculations. If  $nmax1 = nmax2$  ( $=nmax$ ) the calculations are performed once. The variation of  $nmax$  is envisaged only if one desires to study the convergence of the results as a function of the number of the basis states.
- $pi$  is the pi number (3.1415927410125d.0)
- If  $kkind=1$ , calculations are made for the neutrons case.  
If  $kkind=2$ , calculations are made for the protons case.  
Any other value of the  $kkind$  parameter involves an error declaration of the program.
- $Iz$  = number of protons.
- $In$  = number of neutrons.
- $Betta$ , and  $gama$  are the usual deformation parameters of Bohr (eq.(18a)-(18c)).
- If  $ibase=0$  the states of the basis are selected according to the spherical criterion (45).  
If  $ibase=1$ . The states of the base are selected according to the deformed criterion (46) There is not other value for this parameter.
- If  $i1i2=1$ , the program gives all eigenvalues, without eigenvectors.  
If  $i1i2=2$ , the program gives the eigenvalues included in a given interval [elow, ehig] with the corresponding (orthonormalized) eigenvectors. Any other value of this parameter involves an error declaration of the program.
- $Elow$  = lower bound of the selected interval.
- $Ehigh$  = higher bound of the selected interval.  
( Naturally, if this interval is sufficiently large it will contain all eigenvalues.

Consequently all eigenvectors will be also given.)

- If *icalc*=0, the parameters of the Woods-Saxon potential are read from the namelist of the second input file parameters.dat.  
if *icalc*=1, the Myers parameters are calculated by the subroutine woodsparm.
- If *iscal*=1 the basis parameter  $\hbar\omega_0$  is computed from (52) i.e. from  $\hbar\omega_0 = 0.979 |V_0| .A^{-1/3}$   
If *iscal*=2 the basis parameter  $\hbar\omega_0$  is computed from the relation  $\hbar\omega_0 = faktor.A^{-1/3}$ .(see eq.(51).
- *faktor*= input parameter of the previous relation

### 10.1.2 The second input data file: parameters.dat

There is an option ( governed by the keyword *icalc* ) in the first input file which permits to the user to employ its own parameters instead of those of Myers.

The data of the file parameters.dat are :

- *v0neut*= deep of the central part of the potential for the neutrons
- *avneut*= diffuseness of the central part of the potential for the neutrons
- *rvneut*= radius of the central part of the potential for the neutrons
- *capasoneu*= spin-orbit coupling strength for the neutrons
- *assoneu*= diffuseness of the spin-orbit part of the potential for the neutrons
- *rssoneu*= radius of the spin-orbit part of the potential for the neutrons
- *v0pro*= deep of the central part of the potential for the protons
- *avpro*= diffuseness of the central part of the potential for the protons
- *rvpro*= radius of the central part of the potential for the protons
- *capasopro*= spin-orbit coupling strength for the protons
- *assopro*= diffuseness of the spin-orbit part of the potential for the protons
- *rssopro*= radius of the spin-orbit part of the potential for the protons
- *rchpro*= radius of the coulomb potential

### 10.2 The output data

The global results can be extracted from the five arrays *evalplus*, *evalminus*, *evvecplus*, *evvecminus*, and *energies*, in the main program.

The arrays *evalplus* and *evalminus* contain respectively, the eigenvalues for the positive parity and the negative parity . The eigenvalues are classified in an increasing order.

In the same way, the arrays *evvecplus* and *evvecminus* contain the components of the eigenvectors, in columns, in the same order as that of the eigenvalues.

For the positive parity ( respectively the negative parity ) , the parameter *nevalplus* in the subroutine diagoplus (respectively *nevalminus* in the subrou-

tine diagominus) gives the number of eigenvalues.

Sometimes, it is more convenient to gather all eigenvalues in a common array (but the eigenvectors remain in their respective blocks). This is carried out in a common array named *energies*. In this array, the eigenvalues are classified in an increasing order.

In order to find the corresponding eigenvector to a given eigenvalue, a vector containing a supplemental information was created and named *num(k)*. The sign and the absolute value of num(k) indicate respectively the block (i.e. evecplus or evecminus) and the place of the column in this block.

Furthermore, the output data can be consulted in a straightforward way, in three files:

- a) The eigenvalues are written in the file " eigvals.res ". In this file, it is indicated in particular, if the eigenvalues belong to the set corresponding to the positive parity or those corresponding of the negative parity.
- b) The eigenfunctions are recorded in the file " vekt.res ". For every eigenvalue there is a set of components relative to the different states (nx, ny, nz, sigma) of the basis.
- c) A brief study on the convergence is made in the file " conver.res ".

## 11 Checking of the computer code and comments on the test run

In order to check the code, one has proceeded to three types of tests. In the first, we use well-known analytical results. In the second, we compare our calculations with those using the same model. At last, in the third, we use some well-known properties of symmetry.

### 11.1 Analytical tests

In fact, the method of resolution of the Schrodinger equation proposed here is a *purely numerical method*. Consequently, one can use, not only the Woods-Saxon potential, but also *any other type of potential*. It is then possible to replace the Woods-Saxon potential by that of the harmonic oscillator in order to test the code by well-known analytical results.

#### 11.1.1 The deformed case without spin-orbit term

Indeed, for a pure deformed harmonic oscillator, (without spin-orbit interaction), in cartesian coordinates, the theoretical expression of the energy is given simply by:

$$E(n_x, n_y, n_z) = (n_x + \frac{1}{2})\hbar\omega_x + (n_y + \frac{1}{2})\hbar\omega_y + (n_z + \frac{1}{2})\hbar\omega_z$$

$$n_x, n_y, n_z = 0, 1, 2, \dots, \infty$$

For reasons of simplicity, we have chosen the same frequencies as those of the basis. The numerical values are extracted from the file "eigvals1.res".

In the computer program, one must replace the Woods-Saxon potential by that of the harmonic oscillator, i.e. by:

$$V(\vec{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$$

Then, one has to cancel the spin-orbit interaction (by making the function  $\text{potenso} = 0$  or by cancelling the spin-orbit coupling constant) in the code.

Calculating some levels analytically, and comparing them with those of the code, one can note an excellent agreement (to seven significant digits) for the deformed case (see table 1)

It is important to note that the matrix elements are integrated numerically in the computer code, therefore, from this test, we can conclude that the program performs this task correctly. Because this term is diagonal ( in fact the code "does not know this" but after calculations, it finds that the nondiagonal elements are equal to zero ) in our basis, this test does not permit us to verify the diagonalization. These latter part of the program will be verified in the subsections below.

Now, if we add the spin-orbit interaction, we could test the program entirely. Unfortunately, in the deformed case, there is no theoretical expression for that.

### 11.1.2 The spherical case without, and, with spin-orbit term

Of course, for the spherical case, it is possible to make  $\hbar\omega_x = \hbar\omega_y = \hbar\omega_z = \hbar\omega_0$  in the previous theoretical expression. Nevertheless, the spherical coordinates are more convenient because as we shall see, the spin-orbit term has to be "treated" in that system. In this latter, the theoretical expression of the energy of a pure oscillator is well-known:

$$E(n, l, m) = \left[2(n-1) + \ell + \frac{3}{2}\right] \hbar\omega_0 = \left[N + \frac{3}{2}\right] \hbar\omega_0$$

$N = 2(n-1) + \ell =$  This number specifies a major shell

$$n = 1, 2, \dots, \infty$$

$$\ell = 0, 1, 2, \dots, \infty$$

$$m = -\ell, -\ell + 1, \dots, \ell, \quad (\text{for a fixed } \ell)$$

Due to the fact that the spherical symmetry is a particular case of the deformed case, it is obvious, that the results of the code (eivals2.res ) should be in complete agreement ( with the awaited degeneracy) with the analytical results. We can see in table 2a, that it is really the case.

Furthermore, there, contrary to the deformed case, it is possible to obtain the analytical expression for the spin-orbit term.

Indeed, one can use the relation (22) in a suitable way in order to obtain a simple theoretical expression for the spin-orbit term.

Taking  $S(\vec{r}) = cr^2/2$ , where  $c$  is a positive constant, one gets then:

$$-\frac{1}{r} \frac{\partial S(r)}{\partial r} \vec{\ell} \cdot \vec{\sigma} = -c \vec{\ell} \cdot \vec{\sigma} = -2c \vec{\ell} \cdot \vec{s} = -2c \frac{1}{2} (\vec{j}^2 - \vec{\ell}^2 - \vec{s}^2)$$

The most important point is that, in this way the splitting of the major shells does not depend on  $r$ , and, is then *rigorously* given by:

$$\Delta E(\ell - \frac{1}{2}) = c.(\ell + 1) \quad \text{if} \quad j = \left| \ell - \frac{1}{2} \right| \quad \text{and} \quad \ell \neq 0$$

$$\Delta E(\ell + \frac{1}{2}) = -c.\ell \quad \text{if} \quad j = \ell + \frac{1}{2} \quad \text{and} \quad \ell \neq 0$$

Thus, the new energies can be written as:

$$E(n, l, j = \ell \mp \frac{1}{2}) = \left[ 2(n-1) + \ell + \frac{3}{2} \right] \hbar \omega_0 + \Delta E(\ell \mp \frac{1}{2})$$

Therefore, the code can be verified in its integrality.

In order to simplify the numerical values of the splitting, we take  $c = 1 \text{ MeV}$ .

Thus, except for the value  $\ell = 0$ , we can see that the levels are simply shifted by integer values according to the value of  $\ell$ . In order to illustrate that, we will give two examples:

- Example 1 :

if  $\ell = 1$ , the  $p$  shell with a energy noted  $E(p)$  splits into two subshells according to the two values of  $j$ :

$$\text{for } j = \ell + \frac{1}{2} = 1 + \frac{1}{2} = 3/2,$$

$$E(p3/2) = E(p) - \ell = E(p) - 1 \text{ Mev}$$

$$\text{for } j = \ell - \frac{1}{2} = 1 - \frac{1}{2} = 1/2,$$

$$E(p1/2) = E(p) + (\ell + 1) = E(p) + 2 \text{ Mev}$$

- Example 2:

similarly, if  $\ell = 3$  ( $f$  shell ) one obtains

$$\text{for } j = \ell + \frac{1}{2} = 3 + \frac{1}{2} = 7/2,$$

$$E(f7/2) = E(f) - \ell = E(f) - 3 \text{ Mev},$$

$$\text{for } j = \ell - \frac{1}{2} = 3 - \frac{1}{2} = 5/2,$$

$$E(f5/2) = E(f) + (\ell + 1) = E(f) + 4 \text{ Mev}$$

In the table 2b, we compare all results of the code (eigvals3.res) with those of the analytical expression. Practically, the code ( which works in double precision) gives the exact values to six or seven significant digits for all levels of the spectrum.

This high accuracy is due to the fact that the oscillator potential is a polynome of order two, therefore the Gauss method gives in this case the exact values for all matrix elements.

Of course, these tests are not realistic cases, but they prove that the code runs properly with a high degree of precision.

The case with spin-orbit term is very important because it involves the integral analytical checking of the code. Due to the fact that this operator is not diagonal in the oscillator basis, it proves not only that the code performs correctly all calculations of the matrix elements, but also proves that the step of the diagonalization is done properly.

One also made some additional easy checks (not shown here). For example, by taking a constant potential in the spin-orbit term , one cancels the spin-orbit potential . That was well verified by the code, etc...



## 11.2 Comparisons with similar works

For the deformed Woods-Saxon potential, it seemed to us more convenient to compare our code with those of the reference [2]. The reasons are the following:

- a) We use exactly the same model as this reference.
- b) All potential parameters of the calculations are precised in that reference, and we need to use the same.
- c) Not only a part, but the entire spectrum of eigenvalues is given (as a function of the deformation).

The only disadvantage is that the results are displayed under a graphical form. However, in extracting the numerical values, we have tried to minimize the errors by using a graphical software.

The eigenvalues are read with the own scale of the software. Then, a suitable linear transformation returns these values in MeV. Nevertheless, in order to find the "best values", this transformation has been carried out by the least-squares' method of the software.

It turns out that it is possible to obtain values with an error about  $\pm 0.03 \text{ MeV}$ . We have thus considered the deformation ( $\beta = 0.3, \gamma = 0.0$ ) for the lead Pb208. For the basis parameters ( $N_{max}$  and  $\hbar\omega_0$ ), we tried to use in calculations, the same, in order to obtain, as much as possible, close results. For  $N_{max}$ , the reference [2] indicates that the matrices corresponding to the two parities have a dimension of about 160 states. Consequently the fixed value for  $N_{max}$  was certainly  $N_{max}=10$ . However, the value of  $\hbar\omega_0$  really used by the code is not given. This reference indicates only that, for the spherical case, the theoretical relation  $\hbar\omega_0 = 55.A^{-1/3}$  is better than the standard theoretical relation  $\hbar\omega_0 = 41.A^{-1/3}$ . Nevertheless, the reference [9], claims that a practical value of the order of 45-48 MeV (instead 55 MeV) gives a somewhat better results than these theoretical relations. Since the codes of these two references have been compared, it is probable that a common practical value was fixed. We endeavored "to guess" this value. After many tests, It turned out that the value 47 MeV gave a good agreement.

Our calculations were carried out successively with  $N_{max} = 10$  (as the cited reference), and  $N_{max} = 26$ . Indeed, this latter value insures that the levels are calculated with about three or four significant digits near the fermi level, and obviously, all the more for lower levels (see the file "conver13.res"). They are thus practically independent of the choice of the basis parameters.

In the tables (3a-3b, 4a-4b) which have been deduced from the files "eigvals4.res", "eigvals5.res", "eigvals6.res", "eigvals7.res", we show respectively all bound levels of the Pb208 for four cases:

- a) *neutrons-prolate shape* ( $\gamma=0^\circ, \beta = 0.3$ ),  $N_{max}=10$
- b) *protons-prolate shape* ( $\gamma=0^\circ, \beta = 0.3$ ),  $N_{max}=10$
- c) *neutrons-prolate shape* ( $\gamma=0^\circ, \beta = 0.3$ )  $N_{max}=26$
- d) *protons-prolate shape* ( $\gamma=0^\circ, \beta = 0.3$ )  $N_{max}=26$

The levels were separated in two distinct blocks according to their parity. Of course, for a finite potential, the discrete positive energy levels do not represent, a valid solution of the continuum (see ref.[10]), therefore, we shall drop them .

In all cases, we can note that the energy levels are practically the same ones for the low part of the spectrum, but relative small differences appear in the *upper part of the spectrum*.

These differences are more pronounced for  $Nmax = 26$  than for  $Nmax = 10$ . The analyse of these results leads to the following conclusions:

- The lowest levels of the spectrum converge systematically more quickly than the others. As one goes up in the spectrum the convergence is in general slowest, but there can be some rare exceptions.
- A rapid convergence involves a weak dependence relatively to the basis parameters. The highest levels of the spectrum are thus more sensitive to the basis parameters. One can affirm that if the basis parameters of our code are close to those of the reference [2], they are not rigorously the same ones.
- In fact, one noted that this remark is general. Indeed, a modification of any parameter (for example those of the potential) in the calculations produces a modification relatively more significant for the highest levels than for the lowest levels. For example if the radius of the mean potential (spherical case for the neutrons) varies from 7.36fm to 7.40fm (all other parameters being constant), the first level, and the Fermi level undergo variations of 0.05MeV, and 0.28MeV respectively. The "general rule" is thus that *the lowest levels are most "stable"*.
- Owing to the fact that we employ very similar parameters, our results with  $Nmax = 10$  are "artificially" very close to those of the reference [2](the mean deviations are about 0.05 MeV for all cases). Thus, our purpose which was to recover the same results is now reached. But, the word "artificially" means that for this small basis, both results are not enough accurate, although they are the same

Indeed, it is clear that they will be actually less precise than those obtained with  $Nmax = 26$ . Significant differences appear in the top of the spectrum. In the file "conver13.res", one can note that the Fermi level is stabilized to about  $0.01 \sim 0.03 \text{ MeV}$  only starting from  $Nmax = 15 \sim 16$ . Therefore, calculations with  $Nmax = 10 \sim 14$  produce mediocre results.

The rapid convergence of the lowest states is due mainly to the fact that the corresponding wave functions are very similar to those of the oscillator. This is not the case for the highest states where the wave functions are strongly oscillating, and where the edge effect of the potential is "felt".

This can be easily noticed in the components of the eigenvectors, in the file "vekt14.res" . For example, concerning the first eigenvalue, only the compo-

nents corresponding to the lowest quantum numbers are important (see the components numbered 1, 2, 12, and, 59).

### 11.3 Tests using some properties of the parametrisation $(\beta, \gamma)$

Two simple tests can be carried out to check the consistence of the program:

In the first, one compares the spectra obtained with the deformations  $(\beta, \gamma)$  and  $(\beta, -\gamma)$ . This operation is in fact nothing other than a simple permutation of the axes 1 and 2 of the ellipsoid. Of course the two shapes are the same, consequently, the respective spectra must be identical.

In the files "eigvals8.res" and "eigvals9.res" one can easily check that is really the case with an astonishing precision. In particular, one can note in these files the permutation of values of the parameters  $\hbar\omega_x(\text{hbaromegx})$ , and  $\hbar\omega_y(\text{hbaromegy})$ .

In the second, one compares the spectra obtained with the deformations  $(\beta, \gamma = 60^\circ)$  and  $(-\beta, \gamma = 0^\circ)$ . There also, this operation is simply a cyclic permutation of the three axes of the ellipsoid. Therefore, the spectrum must also remain unchanged.

As for the previous case, this can be easily verified in the files "eigvals10.res" and "eigvals11.res".

### 11.4 Tests of convergence

In the files "conver12.res" and "conver13.res", we have shown the convergence of the sum (of the single particle energy) of the first 126 neutrons levels of Pb208 for two deformations. The potential's parameters are those of the reference [2].

This sum has converged to less than 1 MeV only starting from the values  $N_{max} = 14$  and  $N_{max} = 16$ , respectively for the spherical and the deformed cases.

This implies for the Fermi level, a convergence to 0.02 MEV and 0.01 MEV respectively for these two cases. However, for  $N_{max} \sim 16$ , these deviations depend still of the value  $\hbar\omega_0$ . Obviously, for higher bound states, the precision will be less.

Everything depends on what one wants to make. So, for example, for the Strutinsky's shells correction the previous values seem to be sufficient.

Always concerning the Fermi's level (conver13.res), one notices in general that it increases in absolute value as  $N_{max}$  increases, but sometimes, it happens that it decreases slightly (in absolute value). For example, in the spherical case, it passes from 8.510 to 8.502 when  $N_{max}$  passes from 13 to 14. We can easily see that the dimensions of subspaces corresponding to the positive and negative parity do not vary simultaneously when  $N_{max}$  varies by one unit. For example, when one passes from  $N_{max}=13$  to  $N_{max}=14$  only one subspace, namely the one with a positive parity, undergoes changes from 252 basis states to 372 basis states. The other remains the same with 308 basis states.

In our example, the Fermi level belongs to the subspace of negative parity, therefore, apparently, it should not have to change. In fact, the formulae of the spin-orbit interaction connects the matrix elements of the two subspaces (see eq.34-36). This implies always a slight modifications in the subspace which has not varied, and this must not be assimilated to a noise.

In fact, in this method, the "true noise" has two main sources :

- a) under-estimations of the number of points in the numerical integrations of the matrix elements.
- b) a too small basis or really inadequate values of the basis parameters.

With 30 points of quadrature, a double precision, and a large basis ( $N_{max}$  up to 26) these two problems are here minimized.

## 12 Conclusion

We have elaborated and checked a calculation program solving the equation of Schrodinger for a deformed potential of Woods-Saxon type.

The program appears very rapid, and consequently, it becomes possible to use significant basis sizes.

Calculations with small bases, like those which were carried out in the past with  $N_{max} = 10 \sim 12$  lead to a very poor precision. Our conclusions are corroborated by other works. For example, the ref.[5] has shown for Hartree-Fock calculations that the error in the energy of Pb208 is smaller than 1MeV only for  $N_{max} \geq 16$ . Other examples are given in the ref.[4] which confirm this fact.

Similar codes [6,7] were made in the past, but with the assumption of axial symmetry. To our knowledge, triaxial Woods-Saxon calculations were never really undertaken with significant sizes of the oscillator basis.

## A The Myers parameters

The diffuseness parameters  $a_V$ ,  $a_{so}$ , and the spin-orbit coupling  $\kappa$  are the same as those of the Ref.[1].

$$a_V = 0.66 \text{ fm} \quad (\text{A.1})$$

$$a_{so} = 0.55 \text{ fm} \quad (\text{A.2})$$

$$\kappa = 12 \text{ MeV fm}^2 \quad (\text{A.3})$$

The parameters of central potential, and of the spin-orbit potential, were extracted from the Myers droplet model [3,8]. This theory uses Thomas Fermi's approximation to approach average properties of finite nuclei like the density radii, skin-thicknesses, ..., in terms of neutron and proton numbers.

In this model, two auxiliary quantities are first defined:

$$\hat{\delta} = \frac{\frac{N-Z}{A} + 0.0112 \frac{Z^2}{A^{5/3}}}{1 + \frac{3.15}{A^{1/3}}} \quad (\text{A.4})$$

$$\hat{\epsilon} = -\frac{0.147}{A^{1/3}} + 0.330\hat{\delta}^2 + \frac{0.00248Z^2}{A^{4/3}} \quad (\text{A.5})$$

The physical significance of these quantities is explained in the Ref.[3]

With help of these quantities, the depth of the mean potentials are written as:

$$V_0(\text{protons}) = -52.5 - 48.7\hat{\delta} \quad (\text{A.6})$$

$$V_0(\text{neutrons}) = -52.5 + 48.7\hat{\delta} \quad (\text{A.7})$$

The radii of the central potentials (which are different for protons and neutrons) are expressed by means of the nuclear density radii  $R_0(\text{protons})$ , or,  $R_0(\text{neutrons})$ , and the density diffuseness  $a_V$ :

$$R_V(\text{protons}) = R_0(\text{protons}) \left\{ 1 - \frac{\pi^2}{3} \left( \frac{a_V}{R_0(\text{protons})} \right)^2 \right\} \quad (\text{A.8})$$

$$R_V(\text{neutrons}) = R_0(\text{neutrons}) \left\{ 1 - \frac{\pi^2}{3} \left( \frac{a_V}{R_0(\text{neutrons})} \right)^2 \right\} \quad (\text{A.9})$$

with

$$R_0(\text{protons}) = R_0 + 0.82 - \frac{0.56}{R_0} + 0.22\hat{\delta} \quad (\text{A.10})$$

$$R_0(\text{neutrons}) = R_0 + 0.82 - \frac{0.56}{R_0} - 0.22\hat{\delta} \quad (\text{A.11})$$

$$R_0 = r_0 A^{1/3} (1 - \hat{\epsilon}) \quad (\text{A.12})$$

$$r_0 = 1.16 \text{ fm} \quad (\text{A.13})$$

The radius of the spin-orbits mean field is given in the same way:

$$R_{so} = R_0 \left( 1 - \frac{\pi^2}{3} \left( \frac{a_{so}}{R_0} \right)^2 \right) \quad (\text{A.14})$$

At last, the radius of the charge density is given by:

$$R_{ch} = R_0 - \frac{1}{3} r_0 A^{1/3} \left( \frac{N - Z}{N + Z} - \hat{\delta} \right) \quad (\text{A.15})$$

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